

MOMENT ANALYSIS OF TERTIARY PROTEIN STRUCTURES

5 Abstract of the Disclosure

Techniques for analyzing protein structures, such as a tertiary protein structure, are provided. A centroid of the residue centroids is calculated. The centroid of the residue centroids is used as a spatial origin of a global linear hydrophobic moment. The correlation between residue centroid magnitude and residue solvent accessibility is enhanced. The global linear hydrophobic moment is defined, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment. A method for comparing at least two tertiary protein structures is also disclosed.

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